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Constrained Optimization in L_∞-Norm: An Algorithm for Convex Quadratic Interpolation

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A geometrically convergent algorithm is presented to determine min $\| f^{(2)} \|_\infty$, where f interpolates the given p points $\{(x_i, y_i)\}_1^p$ with increasing x_i's, $f \in C^1$, f is absolutely continuous, $f^{(2)} \in L_\infty[x_1, x_p]$, and f satisfies the additional constraint of being convex. Starting with an easily available lower bound $\underline{K}$, it determines an upper bound $\bar{K}$ and then successively reduces the difference $|\bar{K} - \underline{K}|$ to the desired level of accuracy. For the given $\bar{K}$, $\underline{K}$, and an error tolerance level $\varepsilon > 0$, n iterations, where n is the smallest integer $\geqslant (\ln[\varepsilon/(|\bar{K} - \underline{K}|)]/\ln(0.5))$, will determine a k with $|k - k^*| \leqslant \varepsilon$, where k^* is the optimal value of $\| f^{(2)} \|_\infty$. For clarification, a numerical example and results of an initial computer implementation for $p = 5$, 15, 50, 75, 100, are given. These results suggest the algorithm to be fast and capable of solving problems with large values of p. Moreover, the general approach underlying the algorithm would seem to be applicable to other related problems. © 1991 Academic Press, Inc.

1. INTRODUCTION

Let $F_\infty^{(n)}[a, b]$, $-\infty < a < b < \infty$ be a subset of the real Sobolev space

$$W_\infty^{(n)}[a, b] = \{ f : f \in C^{n-1}[a, b]; f^{(n-1)} \text{ abs. cont.}; f^{(n)} \in L_\infty[a, b] \},$$

defined by

$$F_\infty^{(n)}[a, b] = \{ f : f \in W_\infty^{(n)}[a, b]; f \text{ convex}; f(x_i) = y_i, i = 1, ..., p \},$$

where $\{ y_i \}_1^p \in R^p$, $\{ x_i \}_1^p \in R^p$ with $p \geqslant 2$, $x_i < x_{i+n}$, $x_1 = a$, $x_p = b$, and all $x_i \in [a, b]$ are given problem data. Then we define the *nth degree* minimization problem as

$$\min \{ \| f^{(n)} \|_\infty : f \in F_\infty^{(n)}[a, b] \}. \tag{1}$$

Such problems have applications in optimization issues in many areas, including operations research [17, 18], statistics [23], control theory

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[15], and numerical analysis [11, 12]. However, in their full generality, many advanced tools seem to be required for analysis of the existence and characterization of solutions of problems similar to (1) [4, 6, 7, 10–12]. Perhaps due to this, many *special cases* have been studied, Glaeser [8], Louboutin [14], Schoenberg [15], Smith [16], Illiev and Pollul [9], and others. Our purpose here is to give a geometrically convergent algorithm for the *quadratic case* $n=2$, under the convexity constraint with increasing x_i's. The quadratic case is important because of the direct relationship of convexity (concavity) of a function f with $f^{(2)}$, and because bounds on $f^{(2)}$ provide error bounds in often used approximations of nonlinear functions.

For example, if $\hat{f}$ is the piecewise linear function resulting from joining the adjacent points $\{(x_i, y_i)\}_1^p$, then a solution f^* of (1) for $n=2$ gives a bound [17] on the function error: $\max_{a \leqslant x \leqslant b} |f^*(x) - \hat{f}(x)| \leqslant \|f^{*(2)}\|_\infty \delta^2/8$, where $\delta = \max_{1 \leqslant i \leqslant p-1} (x_{i+1} - x_i)$. Since we obviously have $\|f^{*(2)}\|_\infty \leqslant \|f^{(2)}\|_\infty$, $\forall f \in F_\infty^2[a, b]$, a solution f^* is used in the error analysis of convex separable programs [17, 18]. Note that in the context of bounds, L_∞ is the more useful norm. Convexity constraints are also required in many applications.

There is substantial work in this general area, see, e.g., [19]; however, the most closely related work on the quadratic case of (1) is in [9, 19]. In [19], for $n=2$, (1) has been transformed to a convex nonlinear programming formulation (with $(p-1)$ variables, $2(p-2)$ nonlinear constraints, and $(p-2)$ upper and lower bounds) which can then be solved by general nonlinear programming algorithms. However, that approach does not explore or exploit the basic properties of the components of the solutions of the problem, as done here, and would result in a large nonlinear program for a high value of p. The algorithm developed here is direct, does not require a nonlinear programming system, and should be able to solve larger problems. In [9] an algorithm to solve (1) for $n=2$ is stated briefly without any computational details. However, it involves 21 different graphs, several graphs having additional subcases in turn. Therefore many different situations have to be considered and the algorithm does not seem to be easily implementable. The algorithm in [5] deals with L_2 norm and additional smoothing constraints, changing the problem fundamentally.

After the preliminaries and the notation in Section 2, our approach begins with the study of the basic properties of the functions which make up the solutions of the problem in Section 3. In the same section, propositions directly leading to the algorithm are given; they form the basis of the algorithm. Section 4 describes the algorithm and discusses its convergence, followed by the report of our preliminary computational experience along with a detailed numerical example in Section 5. Concluding remarks are given in Section 6.

2. Preliminaries

2.1. *A Related Problem*

As given in [19], for degree n and p given points $\{x_i\}_1^p$, $\{y_i\}_1^p \in R^p$, with $a = x_i < \cdots < x_p = b$, let us define

$$\hat{F}^{(n)}[a, b] = \Big\{ f(x) : f(x) \in W_\infty^{(n)}[a, b]; f(x) \text{ nondecreas.};$$

$$\int_{x_i}^{x_{i+1}} f(x)\, dx = (y_{i+1} - y_i) \text{ for } i = 1, ..., p-1 \Big\}.$$

Now observe that $f^*(x)$, a solution of (1) for $n = 2$, where $a = x_1 < \cdots < x_p = b$, can be obtained by a solution of one degree lower and a more tractable problem:

$$\min \{ \| f^{(1)} \|_\infty : f \in \hat{F}^{(1)}[a, b] \}, \tag{2}$$

by $f^*(x) = \int_{x_1}^x \hat{f}^*(x)\, dx + y_1$, where $\hat{f}^*(x)$ is a solution of (2). Clearly the knots of f^* and $\hat{f}^*$ are the same in number and at identical locations on the abscissae. In the following analysis, we work with problem (2) instead of (1) with $n = 2$.

Problem (2) has been used recently [9, 19] to solve (1) for $n = 2$ via mathematical programming techniques.

2.2. *Notation and Definitions*

For convenience, all the notation is given here first.

(a) For any positive integer i, $k \geqslant 0$, $x_i < x_{i+1}$, and the given problem data, let $d_i = (y_{i+1} - y_i)/(x_{i+1} - x_i)$, $k_i = k(x_{i+1} - x_i)/2$, and $H_i = d_i$, $L_i = d_i - k(x_{i+1} - x_i)/2 = d_i - k_i$, $\Delta x_i = (x_{i+1} - x_i)$, $A_i = d_i \Delta x_i = (y_{i+1} - y_i)$. Note that for $k > 0$, $H_i > L_i$, and H_i is independent of k. To emphasize the *value of* k, specially if it is changing, we will write $L_i(k)$ for L_i.

(b) For given real constants a, b, c, let $h[a, b, c]$ define a real affine funtion on R, passing through the point (a, b) and having slope c everywhere. Thus, $h[a, b, c](a) = b$, $h^{(1)}[a, b, c](x) = c$ for all $x \in R$.

(c) For a positive integer i, $x_i < x_{i+1}$ and real s, $k \geqslant 0$; y_i^+, y_i^-; x_i^+, x_i^- both in $[x_i, x_{i+1}]$, we define a pair of continuous piecewise affine functions on a single interval $[x_i, x_{i+1}]$,

$$\begin{aligned} g_i^+[s, k] &= \begin{cases} h[x_i, s, k](x), & x_i \leqslant x \leqslant x_i^+, \\ h[x_i^+, y_i^+, 0](x), & x_i^+ \leqslant x \leqslant x_{i+1}; \end{cases} \\ g_i^0[s, k] &= \begin{cases} h[x_i, s, 0](x), & x_i \leqslant x \leqslant x_i^0, \\ h[x_i^0, y_i^0, k](x), & x_i^0 \leqslant x \leqslant x_{i+1}; \end{cases} \end{aligned} \tag{3}$$

where $h[x_i, s, k](x_i^+) = y_i^+$, and $h[x_i, s, 0](x_i^0) = y_i^0$, ruling out any jumps in $g_i^+[s, k]$, $g_i^0[s, k]$ at x_i^+, x_i^0, respectively. For referring to both $g_i^+[s, k]$ and $g_i^0[s, k]$, we will omit the sign and use $g_i[s, k]$, or simply g_i. The values x_i^+, y_i^+, x_i^0, y_i^0 are determined by certain conditions to be satisfied by g_i's, often the condition that the mean value be equal to a given constant computed from the data. Note that $g_i^+[s, k]$ ($g_i^0[s, k]$) is a nondecreasing continuous function in $[x_i, x_{i+1}]$ which passes through (x_i, s), has constant slope $k(0)$ from x_i to $x_i^+(x_i^0)$, and 0 (k) after that, and which has at most one knot (the break point in slope).

When $x_i^+ = x_{i+1}$, $x_i^0 = x_i$, we have $g_i^+[s, k] = g_i^0[s, k] = h[x_i, s, k]$ for all $x \in [x_i, x_{i+1}]$, and we will denote this function by $g_i^{++}[s, k]$. Similarly, when $g_i^+[s, k] = g_i^0[s, k] = h[x_i, s, 0]$ it will be written $g_i^{00}[s, k]$.

(d) For the given real values s, $s' < s$, $k \geqslant 0$, positive integers i, $j(j \geqslant i+1)$, $p := j - i + 1$, and a p-point problem data $\{x_r\}_i^j$, $\{y_r\}_i^j$, consider, related to problem (2), the following sets of functions defined in $[x_i, x_j]$:

$$E_{ij}(k) = \left\{ f \in W_\infty^{(1)}[x_i, x_j] : \|f^{(1)}\|_\infty \leqslant k; f(x) \text{ nondecreas. in } [x_i, x_j]; \right.$$

$$\left. \int_{x_r}^{x_{r+1}} f(x)\, dx = y_{r+1} - y_r,\ r = i, ..., j-1 \right\},$$

$$E_{ij}(s, k) = \{ f \in E_{ij}(k) : f(x_i) = s \},$$

and

$$E_{ij}(s', s, k) = \{ f \in E_{ij}(t, k) : t \in [s', s] \}.$$

For a function in any of the above sets it is often convenient to call $f(x_i)$ the *starting* value; $f(x_j)$ the *ending* value; and say that f has *mean values* $d_i, ..., d_{j-1}$, f *covers* $d_i, ..., d_{j-1}$, or $d_i, ..., d_{j-1}$ are *coverable* by f (we may, to emphasize the value of k being used, add *with value* k or *with* k) in $[x_i, x_{i+1}], ..., [x_{j-1}, x_j]$, or, briefly, f *covers* $[x_i, x_j]$. Thus, $f \in E_{ij}(k)$ if it covers $[x_i, x_j]$ with value k; $f \in E_{ij}(s, k)$ if, in addition, it starts at s, and $f \in E_{ij}(s', s, k)$ if it starts somewhere in $[s', s]$.

For these sets of functions, when they are nonempty, and for $i \leqslant r \leqslant j$, we would need the *supremum* and *infimum* values, defined, for example, for the set $E_{ij}(k)$ by $h_{ij}^r(k)$ $(l_{ij}^r(k)) = \sup$ (inf) $\{f(x_r) : f \in E_{ij}(k)\}$. Similar definitions apply for the other sets. These values will be called *extremal* values.

3. Analysis

Using the above notation, first we derive the basic properties of g_i functions.

PROPOSITION 1. *For a given i, $k \geqslant 0$, and a 2-point problem data (x_1, y_1), (x_2, y_2), $x_1 < x_2$ in a single interval $[x_1, x_2]$, the following assertions hold:*

(A) *For any starting value s at x_1, $L_1 \leqslant s \leqslant H_1$, there exist functions $g_1^0[s, k]$, $g_1^+[s, k]$ with mean value d_1 in (x_1, x_2) (i.e., $g_1^0[s, k]$, $g_1^+[s, k]$ both are in $E_{12}(s, k)$), with the properties*

$$g_1^+[s, k](x_2) = \inf\{f(x_2) \in E_{12}(s, k)\},$$
$$g_1^0[s, k](x_2) = \sup\{f(x_2) \in E_{12}(s, k)\};$$

i.e., the ending values at x_2 of these functions, among all the functions with mean d_1 in (x_1, x_2), are the highest and the lowest extremal values (respectively) attainable at x_2.

(B) *For any $s' < s$, $L_1 \leqslant s' < s \leqslant H_1$, and $g_1^+[s, k]$, $g_1^0[s, k] \in E_{12}(s', s, k)$ we have*

$$g_1^+[s, k](x_2) < g_1^+[s', k](x_2),$$
$$g_1^0[s, k](x_2) < g_1^0[s', k](x_2);$$

i.e., $g_1^+[t, k](x_2)$, $g_1^0[t, k](x_2)$ are decreasing functions of t.

(C) *For $s' < s$, $L_1 \leqslant s' < s \leqslant H_1$, $g_1^+[s, k] \in E_{12}(s, k)$, $g_1^0[s', k] \in E_{12}(s', k)$ and any $\bar{t} \in [l := g_1^+[s, k](x_2), h := g_1^0[s', k](x_2)]$, there exists an $\bar{s} \in [s', s]$ and a nondecreasing function g such that $g \in E_{12}(\bar{s}, k)$, $g(x_2) = \bar{t}$ and $g(x_1) = \bar{s}$; i.e., for any ending value in $[l, h]$ at x_2, there is a starting value $\bar{s}$ at x_1 such that a function g with mean d_1 in (x_1, x_2) has three values as its starting and ending values.*

Proof. (A) It is easy to see that if $s = H_1$, then we have $g_1^0[L_1, k] = g_1^+[L_1, k] = g_1^{00}[L_1, k]$ in $[x_1, x_2]$, and if $s = L_1$ then $g_1^0[H_1, k] = g_1^+[H_1, k] = g_1^{++}[H_1, k]$ in $[x_1, x_2]$; in these cases, the break points x_1^+, x_1^0 are at x_1 or x_2. With more details, we can show that as $s = L_1$ increases to some intermediate value in $[L_1, H_1]$, x_1^+, x_1^0 values move to the interior of $[x_1, x_2]$, giving a function with mean value d_1 in (x_1, x_2), as desired. To show that $g_1^+[s, k](x_2) = \inf\{f(x_2) : f \in E_{12}(s, k)\}$, assume there is a $g \in E_{12}(s, k)$ such that $g(x_2) < g_1^+[s, k](x_2)$. We will show that this leads to a contradiction. Since $\int_{x_1}^{x_2} g(x)\, dx = d_1 = \int_{x_1}^{x_2} \bar{g}(x)\, dx$, where $\bar{g} := g_1^+[s, k]$ (for brevity), and $g(x_2) < \bar{g}(x_2)$, there must be a neighborhood where some $\hat{x} \in (x_1, x_2)$ is such that $g(\hat{x}) > \bar{g}(\hat{x})$. If $\hat{x}$ is in $(x_1, x_1^+]$, then the slope of the line through (x_1, s) and $(\hat{x}, g(\hat{x}))$ is larger than k, thus $\| g^{(2)} \|_\infty$ cannot be $\leqslant k$; i.e., $g \notin E_{12}(s, k)$, a contradiction. Similarly, if $\hat{x}$ is in (x_1^+, x_2), consideration of the points $(\hat{x}, g(\hat{x}))$ and $(x_2, g(x_2))$ leads to the conclusion that g cannot be nondecreasing in

$(\hat{x}, x_2)$, hence again $g \notin E_{12}(s, k)$. One can similarly prove the assertion about $g_1^0[s, k](x_2)$.

(B) One can actually show that $g_1^+[t, k](x_2), g_1^0[t, k](x_2)$ as functions of t are *continuous and decreasing*, from which the conclusions follow. For brevity, we simply indicate why the *given* assertions are true. Consider $g_1^+[s, k]$. Since $s > s'$, $g_1^+[s, k]$ starts off at a higher value than $g_1^+[s', k]$ by definition. Now since both have mean value d_1 in (x_1, x_2), there must be, (as in (A) above), an $\hat{x}$, where $g_1^+[s, k](\hat{x}) < g_1^+[s', k](\hat{x})$. But by the definitions of these functions, they change slope only once from k to 0; therefore, $g_1^+[s, k](x)$ must be less than $g_1^+[s', k](x)$, for all $x \geqslant \hat{x}$, hence in particular at x_2.

(C) There are two situations that can arise.

(i) When $\bar{t} \in [l, h]$ is such that there is an $\bar{s} \in [s', s]$ which gives either $g_1^+[\bar{s}, k](x_2) = \bar{t}$ or $g_1^0[\bar{s}, k](x_2) = \bar{t}$ where both the functions have mean d_1 in (x_1, x_2). That is, $\bar{t}$ value is attainable at x_2 by one of the g_i functions, starting off appropriately at x_1.

(ii) When $\bar{t}$ is such that $\bar{s}$ *in* (i) above does not exist. In this case, g is more complicated and has two break points, switching from k to 0 to k, or from 0 to k to 0. Details are lengthy but easy. We will just note that one of the following functions with $\bar{s}$ as either s or s' will always suffice:

$$g(x) = \begin{cases} g_1^+[s, k](x), & x_1 \leqslant x \leqslant \bar{x}_1, \\ h[\bar{x}_1, \bar{s}_1, 0](x), & \bar{x}_1 \leqslant x \leqslant \bar{x}_2, \\ h[\bar{x}_2, \bar{s}_1, k](x), & \bar{x}_2 \leqslant x \leqslant x_2; \end{cases}$$

$$g'(x) = \begin{cases} g_1^0[s', k](x), & x_1 \leqslant x \leqslant \bar{x}_1, \\ h[\bar{x}_1, \bar{s}_1, k](x), & \bar{x}_1 \leqslant x \leqslant \bar{x}_2, \\ h[\bar{x}_2, \bar{s}_1, 0](x), & \bar{x}_2 \leqslant x \leqslant x_2, \end{cases}$$

where $\bar{x}_1, \bar{x}_2, \bar{s}_1, \bar{s}_2$ are such that g and g' have mean d_1 in (x_1, x_2) and are continuous in (x_1, x_2) ∎

The following two useful corollaries follow from Proposition 1.

COROLLARY 1. *To reach the highest (lowest) extremal value at x_2, start at the lowest (highest) extremal value at x_1 and use the $g_1^0[s', k](g_1^+[s, k])$ function.*

COROLLARY 2. *Let the highest and lowest extremal values at x_i be $h := h_{1i}^i(k)$, $l := l_{1i}^i(k)$, respectively, for an i-point problem, then*

$[l, h] \cap [L_i(k), H_i] \neq \phi$ *if and only if* d_i *is* coverable *with value* k *(or* k *is* feasible *for the* $(i+1)$*-point problem).*

The above basic properties of the $g_i^+[s, k]$, $g_i^0[s, k]$ functions, clearly the underlying components of the solutions of the problem, can be used in several ways to analyze the problem. In [21], *without* the convexity constraint, they are used to characterize the solutions with respect to the number of knots and perfectness of $f^{(2)}$. Here, we use them to obtain a solution of the problem. The next proposition computes the highest (lowest) extremal ending values.

PROPOSITION 2. *For* $k \geqslant 0$, *and 2-point data* $\{(x_i, y_i)\}_1^2$, *let a starting value* s *at* x_1, $L_1(k) \leqslant s \leqslant H_1$, *be given. Then the ending values at* x_2 *of the functions* $g_1^+[s, k]$, $g_1^0[s, k]$ *both with mean* d_1 *in* (x_1, x_2) *are determined by*

$$g_1^0[s,k](x_2) = \begin{cases} d_1 & \text{if } s = H_1, \\ d_1 + k_1 & \text{if } s = L_1(k), \\ u^+ & \text{if } x_1 \leqslant \hat{x} \leqslant x_2, \\ u^- & \text{otherwise}; \end{cases}$$

$$g_1^+[s,k](x_2) = \begin{cases} d_1 & \text{if } s = H_1, \\ d_1 + k_1 & \text{if } s = L_1(k), \\ v^+ & \text{if } x_1 \leqslant \tilde{x} \leqslant x_2, \\ v^- & \text{otherwise}; \end{cases}$$

where,

$$u^\pm = s \pm (2k(A_1 - s\Delta x_1))^{1/2},$$
$$\hat{x} = x_2 - ((2A_1 - 2s\Delta x_1)/(u^\pm - s)),$$
$$v^\pm = (s + k\,\Delta x_1) \pm (k^2\,\Delta x_1^2 + 2k(s\,\Delta x_1 - A_1))^{1/2},$$
$$\tilde{x} = (2x_2 - x_1) - ((2A_1 - 2s\,\Delta x_1)/(v^\pm - s)).$$

Proof. We will show that the ending value of $g_1^0[s, k]$ is given as stated; the other follows similarly.

The special-start cases $s = H_1$, $s = L_1(k)$ are obvious; for others, one finds, with a bit of algebra, that the slope k such that $\int_{x_1}^{\hat{x}} h[x_1, s, 0](x)\,dx + \int_{\hat{x}}^{x_2} h[\hat{x}, s, k](x)\,dx = A_1$ is given by $k = (y-s)^2/(2A_1 - 2s\,\Delta x_1)$, where y is the ending value we seek. When we solve this quadratic equation in y, we obtain $y = s \pm (2k(A_1 - s\,\Delta x_1))^{1/2}$. When the two values of y are different, which one should we use? This can be answered by computing $\hat{x}$ as given. With some more tedious algebra, we can show that the value of y which gives $\hat{x}$ in $[x_1, x_2]$ is the correct ending value, and when the two values do not coincide one of these values gives $\hat{x} \in [x_1, x_2]$. One can also show that when the two values are the same it gives a unique $\hat{x}$ in $[x_1, x_2]$. The $g_1^+[s, k]$ case is similar except changes in the formulas: $\int_{x_1}^{\tilde{x}} h[x_1, s, k](x)\, dx + \int_{\tilde{x}}^{x_2} h[\tilde{x}, y, 0](x)\, dx = A_1$ gives $k = (y-s)^2/(2y\, \Delta x_1 - 2A_1)$, and then we obtain $y = v^\pm$, and $\tilde{x}$, as given in the statement. ▌

Using the highest (lowest) starting value and the $g_i^+[s, k](g_i^0[s, k])$ function, by Proposition 1, we will obtain the lowest (highest) extremal value at x_{i+1}. The following proposition describes how this process can be repeated over several intervals, starting from the first interval.

PROPOSITION 3. *For a p-point problem and a value $k \geqslant 0$ the extremal values are given by*:

(A) $h_{12}^2(k) = H_1 + k(x_2 - x_1)/2 = d_1 + k_1$, $l_{12}^2(k) = H_1 = d_1$.

(B) *For any i, $i = 3, ..., p$, if*

$$\Omega_{i-1} = [l_{1i-1}^{i-1}(k), h_{1i-1}^{i-1}(k)] \cap [L_{i-1}(k), H_{i-1}] \neq \phi,$$

then k is feasible for i-point problem and the highest (lowest) extremal values at x_i are given by

$$h_{1i}^i(k) = g_{i-1}^0[\bar{l}_{i-1}, k](x_i), \qquad l_{1i}^i(k) = g_{i-1}^+[\bar{h}_{i-1}, k](x_i),$$

where

$$\bar{h}_{i-1} = \min\{h_{1i-1}^{i-1}(k), H_{i-1}\}, \qquad \bar{l}_{i-1} = \max\{l_{1i-1}^{i-1}(k), L_{i-1}(k)\},$$

and can be computed by Proposition 2.

(C) *If $\Omega_{i-1} \neq \phi$ for $i = 3, ..., p$, then all the intervals are coverable with value k and k is* feasible *for the p-point problem. Otherwise, k is* infeasible *(and $h_{1j}^j(k)$, $l_{1j}^j(k)$ are not defined for any $j \geqslant i', ..., p$, where i' is the first (smallest) integer for which $\Omega_{i'-1} = \phi$).*

Proof. (A) In the first interval (x_1, x_2), it is clear by Proposition 1(B), Corollary 1, that the highest extremal point at x_2 is achieved by the starting value $s = d_1 - k(x_2 - x_1)/2$ at x_1 and using $g_1^{++}[s, k]$ function with mean d_1, which gives $h_{12}^2(k) = H_1 + k_1 = d_1 + k_1$, as stated. Similarly, the starting value d_1 at x_1 and $g_1^{00}[s, k]$ with mean d_1 in (x_1, x_2) gives $l_{12}^2(k) = H_1$.

(B) By Proposition 1, Corollary 2, if the starting value at x_{i-1} is not in $[L_{i-1}(k), H_{i-1}]$ for some i, then $\Omega_{i-1}(k) = \phi$; i.e., k is infeasible for the the i-point problem, and therefore also for the p-point problem. Thus the main task here is to verify the expressions for $h_{1i}^i(k)$ and $l_{1i}^i(k)$. We consider $h_{1i}^i(k)$.

Considering the interval $[x_{i-1}, x_i]$ and $g^{++}_{i-1}[L_{i-1}(k), k]$, the lowest attainable extremal point at x_{i-1} among all the functions in E_{i-1i}; i.e., among the functions with mean d_{i-1} in (x_{i-1}, x_i), is $L_{i-1}(k)$, by Proposition 1. Now by definition, $l^{i-1}_{1i-1}(k)$ is the lowest extremal value at x_{i-1} for the $(i-1)$-point problem, therefore, since the *lowest* extremal value of a problem has to be greater than or equal to the lowest extremal value of any of its subproblems $(E_{1i}(k) = E_{[1,i-1] \cup [i-1,i]}(k))$, we must have $l^{i-1}_{1i}(k) \geq \max\{l^{i-1}_{1i-1}(k), L_{i-1}(k)\} = \bar{l}_{i-1}$. To see that $l^{i-1}_{1i}(k)$ actually equals $\bar{l}_{i-1}$, we note that Proposition 1 (C) and Corollary 2 imply it. Computing $h^i_{1i}(k)$ is now easy: we know that the lowest extremal point at x_{i-1} is $\bar{l}_{i-1}$, so by Proposition 1 (B), Corollary 1, we use $g^0_{i-1}[\bar{l}_{i-1}, k]$ with mean d_{i-1} in (x_{i-1}, x_i) to attain the highest extremal value at x_i as stated. The expression for $l^i_{1i}(k)$ is obtained similarly. ▌

Using the above propositions, one could also develop a method to compute *good* upper and lower bounds on k^*, the minimal value of $\|f^{(2)}\|_\infty$ for the p-point problem. The algorithm then reduces the difference between them to any desired level of accuracy. However, computations to check feasibility/infeasibility of a given k for a p-point problem (Proposition 3) seem quite short, therefore we would use *easily available* bounds or use the algorithm to generate them. For example, one clearly has a lower bound $\underline{K} = \hat{K} = \max\{|\hat{K}_2|, ..., |\hat{K}_{p-1}|\}$, where $\hat{K}_i$ is $f^{(2)}$ of the second degree polynomial through the three consecutive points (x_{i-1}, y_{i-1}), (x_i, y_i), (x_{i+1}, y_{i+1}), given by [3],

$$\hat{K}_i = 2\,\frac{(y_i - y_{i-1})(x_{i+1} - x_i) - (y_{i+1} - y_i)(x_i - x_{i-1})}{(x_i^2 - x_{i-1}^2)(x_{i+1} - x_i) - (x_{i+1}^2 - x_i^2)(x_i - x_{i-1})}. \tag{4}$$

Similarly, under certain conditions, e.g., [17], the upper bound $\bar{K} = 2\underline{K}$.

4. The Algorithm

Since Proposition 3(C) shows how to check if a given value of k is feasible or not for a p-point problem, it is clear how the algorithm will proceed, once the upper and lower bounds on the optimal value of k have been estimated.

4.1. *Outline of the Algorithm*

(A) *Computing the Upper Bound $\bar{K}$.* As discussed in the last section, $\hat{K}$ is an obvious lower bound. We check, using Propositin 3, if $\hat{K}$ is feasible. If $\hat{K}$ is feasible we are done; $\hat{K}$ is the optimal value. If $\hat{K}$ is not feasible, increase the upper bound $\bar{K}$ to $2\hat{K}$ (or some other multiple >1) and check its feasibility again. We keep increasing $\bar{K}$ as many times as necessary till feasibility is obtained; this $\bar{K}$ is our upper bound. (For efficiency, we also update the lower bound in the process).

(B) *Decreasing* $|\bar{K}-\underline{K}|$ *Difference by Bisection.* For the given level of accuracy ε, we decrease the difference $|\bar{K}-\underline{K}|$ by bisection. We can take $k=(\bar{K}+\underline{K})/2$ and, using Proposition 3, check its feasibility or infeasibility. If this k is feasible, update the upper bound $\bar{K}$ to k; if infeasible, update the lower bound $\underline{K}$ to k. We repeat this process till desired accuracy is achieved.

The step by step details of the algorithm are given below.

4.2. *Algorithm Description*

Let k^* be the optimal value of $\|f^{(2)}\|_\infty$ for the p-point problem.

(A) Compute an upper bound $\bar{K}$ on k^*.

(1) Let $\underline{K}=\hat{K}=\max\{|\hat{K}_2|, ..., |\hat{K}_{p-1}|\}$, where $\hat{K}_i$ is given by (4), put $\bar{K}=\underline{K}$.

(2) Check feasibility of $\bar{K}$ by Proposition 3.

(3) If $\bar{K}$ is feasible, we are completely done, the lower bound $\underline{K}$ is sufficient for the entire problem; therefore it is the optimal value of k^* we seek; stop.

(4) If $\bar{K}$ is not feasible; update the lower bound: $\underline{K}=\bar{K}$ (note, the first time this update does not change the value of $\underline{K}$), increase $\bar{K}$ to $2\bar{K}$, and then take $\bar{K}$ to be the mid value $\bar{K}=(\bar{K}+\underline{K})/2$ (thus, the new $\bar{K}=1.5$ old $\bar{K}$); go to the next step.

(5) Check feasibility of $\bar{K}$ by Proposition 3.

(6) If $\bar{K}$ is feasible, we have computed the upper bound on k^*, go to the next phase (B) of the algorithm with these values of $\bar{K}$ and $\underline{K}$.

(7) If $\bar{K}$ is not feasible, go to step (4).

(B) Decrease initial $|\bar{K}-\underline{K}|$ to obtain final $|\bar{K}-\underline{K}|\leqslant\varepsilon$.

(8) If $|\bar{K}-\underline{K}|\leqslant\varepsilon$, take $k^*=\bar{K}$, stop; otherwise, go to the next step.

(9) Take $k=(\bar{K}+\underline{K})/2$ and check its feasibility for the p-point problem by Proposition 3. If k is feasible, go to the next step; otherwise, go to step (11).

(10) k is feasible for the p-point problem. If $|k-\underline{K}|\leqslant\varepsilon$, take $k^*=k$, stop; otherwise, update (*decrease*) the upper bound $\bar{K}=k$, and go to step (9).

(11) k is not feasible for the p-point problem. If $|\bar{K}-k|\leqslant\varepsilon$, take $k^*=\bar{K}$, stop; otherwise, update (*increase*) the lower bound $\underline{K}=k$ and go to step (9).

4.3. *Convergence*

As discussed earlier (at the end of Section 3), computations to check feasibility seem quite simple and fast, and once we have obtained the bounds $\underline{K}$, $\bar{K}$, the well-known bisection procedure of (B) above gives final $|\bar{K}-\underline{K}| \leqslant \varepsilon$ in n iterations, where n is the smallest integer implying $(.5)^n \leqslant \varepsilon/(\bar{K}-\underline{K})$ for the *initial* values of $\underline{K}$ and $\bar{K}$ [1, 2, 3].

5. Computational Work

5.1. *A Numerical Example*

To clarify the algorithm we take a 4-point problem $\{x_i\}_1^4 \equiv \{0, 1, 2, 3\}$, $\{y_i\}_1^4 \equiv \{1, 4, 13, 24\}$. It can be shown (with some work) that k^*, the minimal $\|f^{(2)}\|_\infty$ of the convex spline, is 6.111456, or $(32/(3+\sqrt{5}))$ to be exact, (if the convexity constraint is dropped, k^* is only 6). By (4), we have $\hat{K}_2 = 6$, $\hat{K}_3 = 2$. Now we follow the algorithm steps *given in Section* 4.2.

(A) *Computing the upper bound.*

(1) The lower bound $\underline{K} = \max\{\hat{K}_2, \hat{K}_3\} = 6$, take also $\bar{K} = 6$.

(2) Check feasibility of $k=6$, using Proposition 3: $h_{12}^2(6) = d_1 + k(x_2 - x_1)/2 = 3 + 6(1/2) = 6$, $l_{12}^2(6) = d_1 = 3$; by definition $L_2(6) = d_2 - k(x_3 - x_2)/2 = 9 - 6(1/2) = 6$, $H_2 = 9$; thus $\Omega_2(6) = [l_{12}^2(6), h_{12}^2(6)] \cap [L_2(6), H_2] = [3, 6] \cap [6, 9] = \{6\} \neq \phi$, and therefore $k=6$ is feasible for $(i=3)$-point problem. Now let us check if it is feasible in the next interval. We first compute the ending extremal values at $x_3 : \bar{l}_2 = \max\{l_{12}^2(6), L_2(6)\} = \max\{3, 6\} = 6$, $\bar{h}_2 = \min\{h_{12}^2(6), H_2\} = \min\{6, 9\} = 6$, therefore the ending extremal values at x_3 are given by $h_{13}^3(6) = g_2^0[\bar{l}_2, 6](x_3) = g_2^0[6, 6](2)$, and $l_{13}^3(6) = g_2^+[\bar{h}_2, 6](x_3) = g_2^+[6, 6](2)$. Computing these values by Proposition 2, we obtain, since $s = 6 = L_2(6)$, $h_{13}^3(6) = l_{13}^3(6) = d_2 + k_2 = d_2 + k(x_3 - x_2)/2 = 9 + 6(1/2) = 12$. By definition, $L_3(6) = d_3 - k(x_4 - x_3)/2 = 11 - 6(1/2) = 8$, $H_3 = d_3 = 11$. Now, since $\Omega_3(6) = [l_{13}^3(6), h_{13}^3(6)] \cap [L_3(6), H_3] = [12, 12] \cap [8, 11] = \phi$, $k=6$ is *not* feasible for the $(i=4)$-point problem, and we go to step (4).

(4) Update $\underline{K} = \bar{K} = 6$ (unchanged in the first iteration), increase $\bar{K} = 2\bar{K} = 12$, then take the mid value $\bar{K} = (\bar{K} + \underline{K})/2 = (6+12)/2 = 9$, and go to step (5): checking feasibility of $\bar{K} = 9$ by Proposition 3. As done above, we find $\Omega_2(9) = [l_{12}^2(9), h_{12}^2(9)] \cap [L_2(9), H_2] = [3, 7.5] \cap [4.5, 9] = [4.5, 7.5] \neq \phi$, hence $k=9$ is feasible for the 3-point problem (obviously, since $k = 6 < 9$ was feasible before, but we need the computations to proceed any way).

Now $\Omega_3(9) = [l_{13}^3(9), h_{13}^3(9)] \cap [L_3(9), H_3]$ needs to be computed using Proposition 2 and 3. First, $\bar{l}_2 = \max\{l_{12}^2(9), L_2(9)\} = \max\{3, 4.5\} = 4.5$,

$\bar{h}_2 = \min\{h_{12}^2(9), H_2\} = \min\{7.5, 9\} = 7.5$, then $l_{13}^3(9) = g_2^+[\bar{h}_2, 9](x_3) = g_2^+[7.5, 9](2)$ and $h_{13}^3(9) = g_2^0[\bar{l}_2, 9](x_3) = g_2^0[4.5, 9](2)$. The ending values of the g functions are computed by Proposition 2. We illustrate it by computing $g_2^+[7.5, 9](2)$: we find $v^+ = 23.8485$, $v^- = 9.1515$, $\tilde{x}(\text{for } v^+) = 2.8165$, and $\tilde{x}$ (for v^-) $= 1.1835$ (long formulas). The $\tilde{x}$ for v^- is within $[x_2 = 1, x_3 = 2]$, hence $l_{13}^3(9) = v^-$ is the appropriate ending value. Similarly Proposition 2 gives $h_{13}^3(9) = 13.5$, since $s = 4.5 = L_2(9)$. By definition, $L_3(9) = 6.5$, $H_3 = 11.0$. Therefore, $\Omega_3(9) = [9.1515, 13.5] \cap [6.5, 11.0] = [6.5, 11] \neq \phi$, and $k = 9$ is feasible for the 4-point problem; i.e., for the entire problem. Thus we have computed the upper bound $\bar{K}$ for the problem, and we go to the next phase: decrease $|\bar{K} - \underline{K}|$, starting with $\bar{K} = 9$, $\underline{K} = 6$.

(**B**) *Decrease initial* $|\bar{K} - \underline{K}|$ *to obtain final* $|\bar{K} - \underline{K}| \leqslant \varepsilon$. Since all the basic computing steps—(i) $L_i(k)$, H_i, (ii) $l_{1i}^i(k)$, $h_{1i}^i(k)$ via $g_{i-1}^+[\bar{h}_{i-1}, k]$, $g_{i-1}^0[\bar{l}_{i-1}, k]$, v^+, v^-, $\tilde{x}(v^+)$, $\tilde{x}(v^-)(u^+, u^-, \hat{x}(u^+), \hat{x}(u^-)$, are analogous) of Proposition 2, and (iii) $\Omega_i(k)$ of Proposition 3—have been illustrated above, only the summary of the iterations is given in Table I.

Let $\varepsilon = 0.1$, then at step (8), $|\bar{K} - \underline{K}| \nleqslant \varepsilon$ and we take $k = (\bar{K} + \underline{K})/2 = (9 + 6)/2 = 7.5$. This value is found to be feasible and the next value of k is 6.75. The value of k decreases till $k = 6.09375$, when it is found to be *infeasible* in iteration 5, and we have $|\bar{K} - \underline{K}| = |6.1875 - 6.9375| \leqslant \varepsilon = 0.1$. Since $(\ln(\varepsilon/|\bar{K} - \underline{K}|)/\ln(.5)) = \ln(.033333)/\ln(.5) = 4.906$; $n = 5$ (the smallest integer $\geqslant 4.906$) iterations are guaranteed to obtain for us $|\bar{K} - \underline{K}| \leqslant 0.1$. With some more iterations (not shown in Table I but as for all the examples in the next section), accuracy within $\pm\varepsilon = 0.00001$ is achieved.

5.2. *A Computer Implementation*

We implemented the algorithm using FORTRAN 77, and tested the program on an IBM3090, under CMS. The optimal solution k^* was known geometrically for the smaller problems. For the larger problems, the given (or randomly generated) x_i values and locations of the knots are used to compute the y_i values (by integration) such that a specified value of k^* is optimal. The CPU times for different size problems are given below.

Problem size

No. of points p	5	15	50	75	100
CPU Secs.	1.6	2.15	4.40	5.9	7.8

In all cases the algorithm determined k^* within $\varepsilon = 0.00001$ in 15 to 25 iterations. For these problems, the computation times are small and appear to increase rather slowly (linearly or less); indicating that the algorithm is efficient and should be able to solve problems for large values of p.

TABLE I

Algorithm Iterations: Decreasing $|\bar{K} - \underline{K}|$

	Initial $\bar{K} = 9$, $\underline{K} = 6$, $k = 7.5$				
	Iteration 1	Iteration 2	Iteration 3	Iteration 4	Iteration 5
k	7.5	6.75	6.375	6.1875	6.09375
$L_2(k)$	5.25	5.625	5.8125	5.90625	6.09375
H_2	9.00	9.00	9.00	9.00	9.00
$l^2_{12}(k)$	3.00	3.00	3.00	3.00	3.00
$h^2_{12}(k)$	6.75	6.375	6.1875	6.09375	6.0469
$\Omega_2(k)$	[5.250, 6.750]	[5.625, 6.375]	[5.813, 6.188]	[5.906, 6.094]	[5.953, 6.047]
$\underline{l}_2$	5.25	5.625	5.8125	5.906	5.9531
$\bar{h}_2$	6.75	6.375	6.1875	6.094	6.0469
Special start	$s = L_2(7.5)$	$s = L_2(6.75)$	$s = L_2(6.375)$	$s = L_2(6.1875)$	$s = L_2(6.0937)$
$h^3_{13}(k)$	12.75	12.375	12.1875	12.094	12.0469
v^+	18.99	16.3070	14.7491	13.8045	13.2095
$\tilde{x}(v^+)$	2.6325	2.4714	2.3430	2.2462	2.1754
v^-	9.5066	9.9430	10.3759	10.7580	11.0717
$\tilde{x}(v^-)$	1.3675	1.5286	1.6570	1.7538	1.8246
$l^3_{13}(k)$	9.5066	9.9430	10.3759	10.7580	11.0717
$L_3(k)$	7.25	7.625	7.8125	7.9063	7.9531
H_3	11.00	11.00	11.00	11.00	11.00
$\Omega_3(k)$	[9.566, 11]	[9.625, 11]	[10.376, 11]	[10.758, 11]	ϕ
k Feas/infeas.	Feasible	Feasible	Feasible	Feasible	Infeasible
Update $\bar{K}$ or $\underline{K}$	$\bar{K} = k = 7.5$	$\bar{K} = k = 6.75$	$\bar{K} = k = 6.375$	$\bar{K} = k = 6.1875$	$\underline{K} = k = 6.09375$
Next $k = (\bar{K} + \underline{K})/2$	$(7.5 + 6)/2 = 6.75$	$(6.75 + 6)/2 = 6.375$	$(6.375 + 6)/2 = 6.1875$	$(6.1875 + 6)/2 = 6.09375$	$\lvert\bar{K} - \underline{K}\rvert \leqslant 0.1$ (Done!)

6. Concluding Remarks

A direct algorithm to get the minimal $\|f^{(2)}\|_\infty$ of a convex quadratic spline which solves problem (1) has been presented. From initial results, computation times from a straight forward implementation look quite encouraging. Since the approach taken is based on (i) the properties of the underlying functions making up the optimal solutions (Proposition 1), and on the results (ii) which compute the extremal ending values (Proposition 2), and (iii) which check the feasibility of a given value of $\|f^{(2)}\|_\infty$ (Proposition 3); it should be applicable to other related problems; e.g., to repeating data and to general quadratic approximation without the convexity (concavity) constraint [22], or with additional constraints besides convexity. Clearly, another interesting question is the applicability of the approach more broadly—to problems of degrees higher than the second degree considered here. Some work in these directions is under way.

The referee has pointed out an interesting connection between the optimal value k^* of the problem with the convexity constraint discussed above and an unconstrained problem. If we replace the y_i values of the constrained problem by shifted values: $(2y_i - x_i^2 k^*/2)$ and solve this problem without the convexity constraint (by an appropriate algorithm), then $F^* = k^*$, where F^* is the optimal solution of the unconstrained problem. Note, however, that this does not allow us to obtain the solution of the constrained problem by solving the unconstrained problem since computation of the shifted values of y_i's requires k^*.

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